

QUICK USER GUIDE

FOR MORE TRAINING MATERIALS VISIT:

www.reaxys.com/info/welcome-pack

HOW DO I...

INSTRUCTIONS

Register for a **password**.



Click the **Register** button in the upper right part of the screen.

Change **password**.



Click the **My Settings** button. Then click the **Change Password** link.

Find out about tested environments involving Windows, Mac, and Java.

Tested Environments

Please note: Reaxys is a web-based application using which support Java 1.5 or higher and JavaScript execut ensure that all features fun in those environments. Using

Windows PC

Macintosh PC

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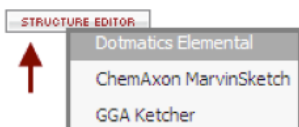
Click the **About Reaxys** link located at the bottom of the Query page.

Find information about the databases included in a Reaxys search.

Sources: [Reaxys](#), [PubChem](#), [eMolecules](#).

Click on one of the hyperlinks towards the top of the Query page to display the info sites for those databases.

Select a Structure Editor.



Click the **Structure Editor** button located in the lower right side of the structure box on the **Query** page. Click the structure box to open the Structure Editor. If you are on the **Start page**, you will first have to click the box on the far left labeled **Substances/Reactions** to open the structure box.

Use these external structure editors:

- **Accelrys ISIS/Draw**
- **ChemDraw**
- **Accelrys/Draw**
- **ICEdit**
- **CrossFire SE**

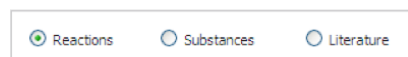


1. Install the external structure editor.
2. Download the **Reaxys Structure Editor Plug-in** from http://www.reaxys.com/info/support_downloads and install it.
Download **ChemDraw/Reaxys Plug-in**:
<http://scistore.cambridgesoft.com/ScistoreProductPage.aspx?ItemID=5943> and install.)
Download the **ICEdit/Reaxys Plug-in** from
<http://www.infochem.de/content/downloads/iceditinreaxys.pdf>
3. Click the **My Settings** button. Then click the **Modify Application Settings** link, select your structure editor and click **Save**.

HOW DO I...

INSTRUCTIONS

Select **Substances** or **Reactions** as the type of search.



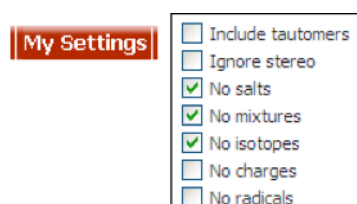
Click the appropriate selection, **Substances** or **Reactions**, located above the structure box on the **Standard** and **Advanced** tab. If you are on the **Start** page, you will first have to click the box on the far left labeled **Substances/Reactions** to view the structure box.

Create a structure from a name CAS#, InChIkey, or smiles string.

Create structure template from name

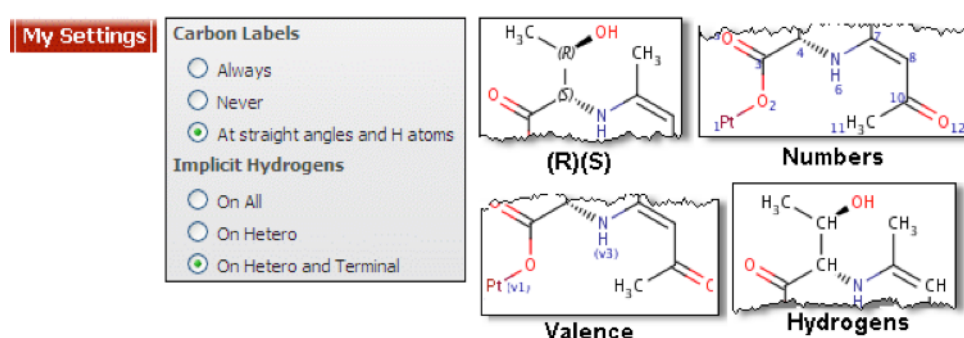
Click the **Create structure template from name** link under the Structure box, type in the query and click **Submit**. (Use the operator dropdown menu, if needed). If several structures share the same name, a list of structures will appear with the most relevant first.

Customize the settings for **reaction or substance search options**.



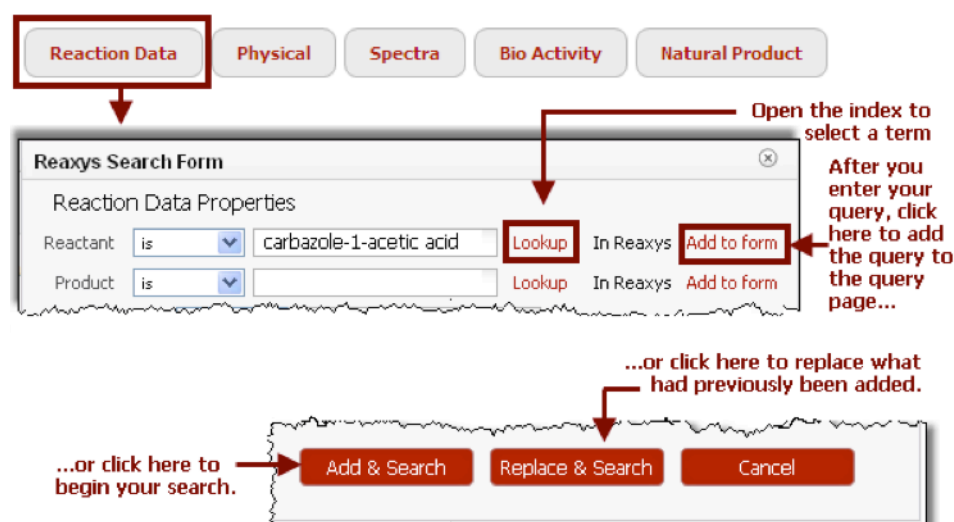
Click the **My Settings** button. Then click the **Modify Application Settings** link and look for **Reaction or Structure Search Options**.

Customize the settings for **structure display options**.



Click the **My Settings** button. Then click the **Modify Application Settings** link and look for **Structure Display Options**.

Display a form so that I can use **keywords** or **data** in my query.



Select a category and click to display the corresponding form. Type in a query or use the **Lookup** table to select an entry. Click **Add to Form** if: 1). your query contains a structure/reaction, 2). You have already entered some data on the Query page, or 3). You plan to add additional data to your query. Click **Replace & Search** if you had previously entered data in a particular field (i.e., it is displayed on the **Query page**). Click **Add & Search** if the data entered on the form contains your complete query, i.e., your query does not already contain a structure/reaction or data, and you do not plan to add any more to the query.

Searching the **Literature** fields together with a structure or reaction will retrieve a list of all substances and all reactions from documents that fit the bibliographic search criteria. If, instead, you wish to do a **Literature search** you can find information here.

Use the **Lookup** tables in the **Data forms**.

The screenshot shows the 'Reaxys Search Form' on the left and a 'Select index items and click 'Transfer'' dialog on the right. The search form has fields for Reactant, Product, Reagent/Catalyst, and Yield, each with a 'Lookup' button. The dialog shows a search for 'tetraacetyl' with a list of results including 'tetraacetyl diborate (141)', 'tetraacetyl riboflavin (17)', and 'tetraacetylriboflavin (35)'. A red arrow points from the 'Lookup' button in the search form to the dialog.

Click the appropriate **Lookup** link to open the index to select specific data. In the index, type in your data. Click to select your data from the list. Use the **Shift** and **Control** keys to make multiple selections. Then click the **Transfer** button to add the data to your form. Click **Add Specified Fields to Query** to add the data to the **Query** page.

Customize a **Data form**.

The screenshot shows the 'Add/Remove Physical Search Fields' dialog. It has a 'Find any property' search box and a 'RESET' button. The left pane lists available properties under 'Reaxys', including 'Melting Point', 'Boiling Point', 'Sublimation', 'Refractive Index', 'Density', and 'Adsorption (MCS)'. The right pane shows the current form's fields, including 'Boiling Point', 'Density', 'Solubility (MCS)', 'Dissociation Exponent', 'Refractive Index', 'Optical Rotatory Power', and 'Partition octan-1-ol/water (MCS)'. Between the panes are 'Add >>', 'Remove', and 'Remove all' buttons. A 'Save' button is at the bottom right. A red arrow points from the 'Save' button to a callout box at the bottom of the dialog.

Add / Remove fields

Buttons: **Add & Search**, **Replace & Search**, **Cancel**

Select a form from the buttons labeled *Identification*, *Reaction*, *Bibliographic*, etc. and click to open it. Then click the **Add/Remove properties** link at the bottom of the form. The **Add/Remove** box is displayed with all of the available fields shown on the left and the fields chosen in your current form on the right. Select a field from the left (use the **Shift** or **Ctrl** keys for multiple selections) and then click the **Add** button (between the left and right columns) to move your selection to the right. (Adjust the placement of the fields in your new list by clicking the arrows on the far right). Click the **Save** button. The new fields will now appear on your form. Fields can be removed in a similar way: click **Add/Remove Properties** and select the fields you want to remove from the right column, click the **middle arrow**, and then click **Save**.

Please note: If you cannot find the field you need on the left, begin typing part of the field name into the entry box next to **Find any property** and the relevant fields will be displayed at the top of the list.

Customize a **Data form**
(continued).

Add/Remove Identification Search Fields

Find any property

Field lists for each database

- Reaxys
- PubChem
- eMolecules
 - Substance Identification
 - eMolecules Compound ID (IDE.EID)
 - Version ID (IDE.VERSIONID)
 - Parent ID (IDE.PARENTID)
 - Compound Type (IDE.CTYPE)
 - CAS Registry Number (IDE.CASRN)
 - EMolecules Link (IDE.LINK)
 - Chemical Name (IDE.CN)
 - Chemical Name Segment (IDE.CNS)
 - Linear Structure Formula (IDE.LSF)
 - Molecular Formula (IDE.MF)
 - Search MF Range (IDE.MOFO)
 - Charge (IDE.CHA)
 - Element Counts (IDE.ELC)
 - Element Symbols (IDE.ELS)

Buttons: Add >>, Remove, Remove all

Selected fields:

- Reaxys Registry Number (in multiple)
- CAS Registry Number
- Chemical Name
- Molecular Formula
- Molecular Weight
- Number of Elements (in multiple)
- Number of Fragments (in multiple)
- Prophetic Compound (in Reaxys)
- Parent ID (in eMolecules)

Tooltip: Reaxys Registry Number (IDE.XRN) is presented in: Reaxys, PubChem, eMolecules

Note: highlighted fields will search in multiple databases

Many fields in **Reaxys** have been mapped to fields in **PubChem** and **eMolecules** and those results appear automatically when you do a substance search. There are also many fields that are unique to **PubChem** and **eMolecules** that can be searched from within **Reaxys**.

For example eMolecules has a unique field for the parent compound identification. This field can be added to your customized form. Notice that in the example above you can hover over a hyperlink on the right side to see which databases contain that field. When the field appears in only one database, the name of the database is shown.

Save a **Data Form**
for future use.

☐ Reactions ☒ Substances ☐ Literature

Create Structure Template from Name

Molecular Weight =

Melting Point (°C) =

NMR Spectroscopy ☒ exists

Effect is

Logical operators: AND, AND, AND, NOT

Categories: Substances / Reactions, Identification, Literature

Buttons: Reaction Data, Physical, Spectra, Bio Activity, Natural Product

Query:

Select the appropriate radio button (*Reactions, Substances, Literature*). Select the desired fields by clicking any of the buttons on the bottom of the **Standard** tab and then clicking **Add to form** near each field. If a field you need does not already appear on the form, click **Add/Remove fields** (see above), and then select the needed fields.

You can mix fields from any of the categories (*Physical, Identification, etc.*). Then click the **Save** button in the top right corner to save the form to your computer. Retrieve the form by clicking the **Import** button (next to the **Save** button.)

Add a **keyword** or **data** to your query using the **Advanced** form.

and/or enter an advanced factual query:

VP.VP='0.306256 - 3.3'

Hide searchable fields Check Syntax

If you don't know the field code, search for a topic here:

enth RESET

Temperature, °C (HHDG.T)

Enthalpy of Sublimation exists

Enthalpy of Sublimation, Jmol⁻¹ (HSP.HSP)

Temperature, °C (HSP.T)

Enthalpy of Vaporization exists

and Enthalpy of Vaporization, Jmol⁻¹ (HVAP.H) = **Lookup**

Temperature, °C (HVAP.T)

Pressure, Torr (HVAP.P)

Search for the field name here

Click to open the index and select data

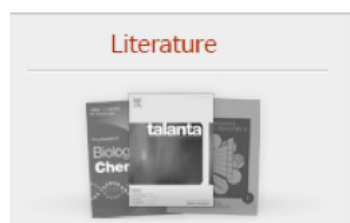
The **Advanced** form gives you access to the data structure so that you can create complex queries using different fields and data operators.

Click the **Advanced** tab. Then click the **Show Searchable Fields** link towards the bottom of the page. Find the appropriate field by typing a partial field name into the box under the words **If you don't know the field code search for a topic here**. Relevant field names will appear as you type. Select the field from the list that appears. Select **exists** for a general search of that field, or click the field name and then click the **Lookup** link to open the index to select specific data. In the index, type in your data. Click to select your data from the list. Use the **Shift** and **Control** keys to make multiple selections. Then click the **Transfer** button.

Please note: If several subfields are listed under a field name, e. g., *boiling point* and *b.p. pressure*, you can use the operator **Proximity** when building your query with these fields. This will ensure that your results are aligned.

The Basic Index fields are for keyword searching. The other fields are for data searching.

Perform **Literature Searching**.



From Start page

Standard Advanced

Reactions Substances **Literature**

Literature

From the Standard tab

Standard **Advanced**

Reactions Substances **Literature**

Bibliographic Data

- Citation Number
- Citation
 - Document Type (CIT.D)
 - Authors (CIT.AU)
 - Patent Assignee (CIT.A)
 - Common Patent Number
 - Patent Country Code

From the Advanced tab

HOW DO I...

INSTRUCTIONS

Perform **Literature Searching** (continued).

To find a list of specific citations *with their associated substances and reactions (if any)*, do any of the following:

- Click the **Literature** picture on the **Start** page to open the **default Literature form**.
- Click the **Literature** radio button on the **Standard tab** and then click the **Literature button** at the bottom to open the **default Literature form**.
- Click the **Literature** radio button on the **Advanced tab** and then click the **Show Searchable Fields** link at the bottom of the page. Scroll to bibliographic Data.

Use the **field at the top of the page** on the **default Literature form** to find keywords or phrases that may be contained in titles, abstracts, or author names. Use wildcards (*) and operators like *and*, *or*, *near* (within a few words), and *next* (adjacent words). Use the **Lookup** link next to each field to search the index.

Click [here](#) for information on using the **Advanced tab**.

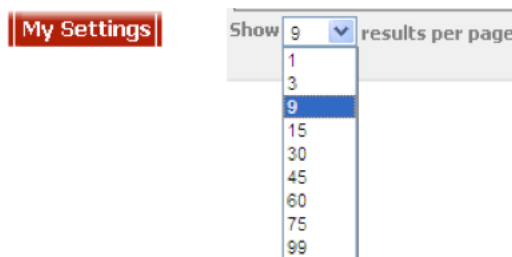
Please Note: Clicking the **Substances** or **Reactions** radio button will allow for **bibliographic searching**, but the results will be structure/ reaction lists with their associated citations and most likely will include additional citations that were not in your query.

Save a query.



Click the **Save** button in the upper right corner of the **Query** tab.

Set the number of hits per page.



Click the **My Settings** button. Then click the **Modify Application Settings** link. To temporarily change the number of hits per page, select the appropriate number from the drop-down menu in the lower left side of the **Results** page.

Change the structure and text highlight colors.



Click the **My Settings** button. Then click the **Modify Application Settings** link.

Change the **size** of **substances** or **reactions**.



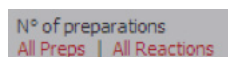
Use the **zoom** buttons on the toolbar on the results page.

Show/Hide reaction or **Substance** details.



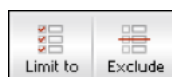
Click the appropriate button on the tool bar on the results page..

Generate a list of associated **reactions** from a **substance** list.



From the **Substances (Table)** results tab, select the link for **All Preps** (substances in the list are products in the reactions) or **All Reactions** (substances in the list can be products or reactants).

Limit results to specific hits.



Click the check-boxes (left side of hit) to select the hits, and then click the **Limit to Selection** button.

HOW DO I...

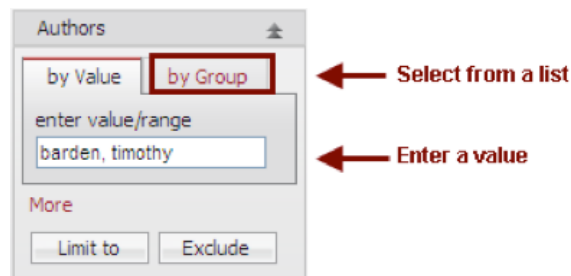
Limit results to hits with specific properties.

INSTRUCTIONS

Filter by:

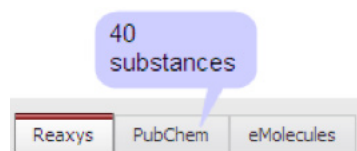
Find the appropriate filter on the left side of the results screen, select properties and click the **Limit** to button. If the word **more** appears at the bottom of the filter, click the **more** link and specify property data in the pop-up box. After filtering, the available data for the hit will include a link called **Hit Data**.

Limit results to a specific author.



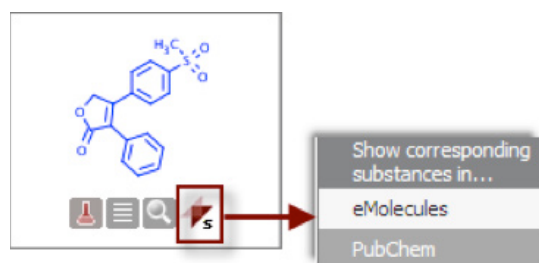
Some filters give you the choice of entering the value or selecting the value from a list. For example, to filter by author, find the appropriate filter on the left side of the results screen, click to select author(s). If the list is very long, clicking the more link will not display the complete list. In this case, click the **By Value** tab in the filter and type in the sname (wildcards can be used).

View the results from different databases.



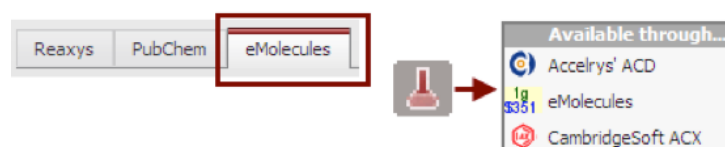
By default, the Reaxys results will be displayed on the **Results** page. You can hover over the tab for other databases to see the number of results and then click the tab to view the results from within Reaxys. If no results were found in Reaxys, the tab for the database with the largest number of hits will automatically be selected.

View a single substance in multiple data-bases.



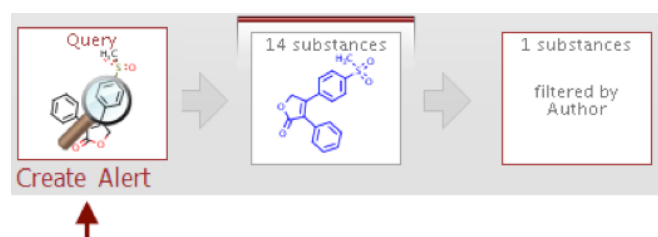
Click the Reaxys logo under a structure and select a database.

View supplier availability and pricing info.



eMolecules pricing and availability information is displayed by clicking the **eMolecules** tab. Click the **flask** icon under a substance to find options for linking to **eMolecules**, a free website, **Accelrys ACD** database (requires a license), and **CambridgeSoft's ACX** (requires a license).

Create an **Alert**.



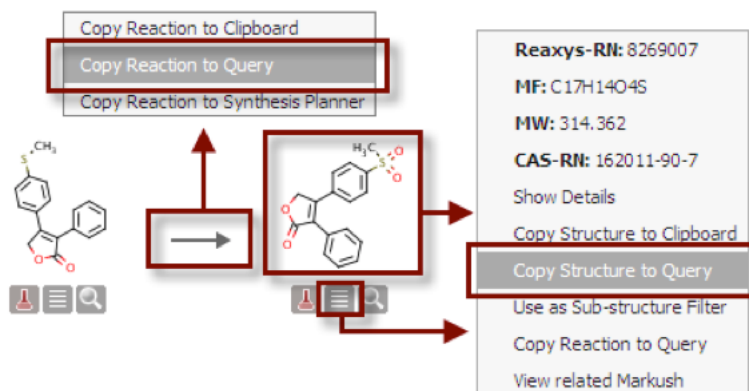
Click the **Create Alert** link under the first breadcrumb in the upper left corner of the results screen or click the **History** button and then click the **Create Alert** link under the query.

Save Results.

History

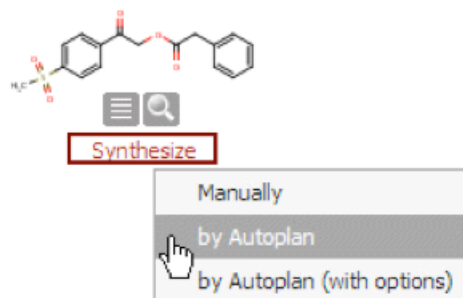
Click the **History** button from the Results page. Then click the **Store** link on the right side of the screen.

Copy a substance or reaction from the Results screen.



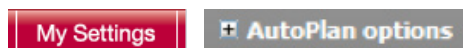
Display the Options **Menu** by clicking the grey box below a substance (or below any substance in a reaction), or click directly on a substance, and select the appropriate option. You can also click the **arrow** in the reaction and then select an option.

Start an **AutoPlan**.



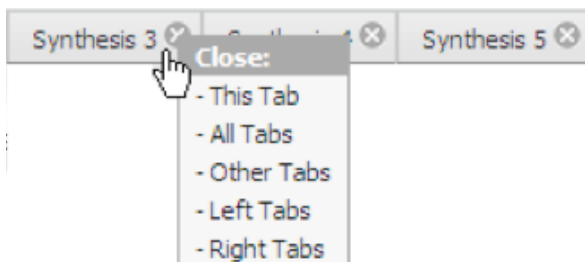
Click the **Synthesize** link under a structure in the results or in the **Synthesis Planner** and select **by Autoplan**.

Select the settings for **Autoplan**.



From the **My Settings** page, click **Modify Application Settings**>**Autoplan options**.

Close tabs in the **Synthesis Planner**.



Click the **Close X** to reveal the options.

Copy a **synthesis plan** to the **Reaxys Report**.



Click the **Report** button on the **Synthesis Planner** tool bar or click the page curl on one of the tabs.

Filter using **histograms**.



From the **Results** page, select the **Open Analysis View** button. Select a category from the dropdown menu of **Histogram A** and then click the desired bins. Analyze the data by comparing it to other categories and bins in **Histogram B**.

HOW DO I...

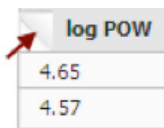
INSTRUCTIONS

Select specific details to copy to the **Reaxys Report**.



To select a detail, look for a page curl image as you hover over details. Click the page curl to see the options specific to that detail and click to select.

Select a whole list of details to copy to the **Reaxys Report**.



A whole list of facts can be copied by clicking the header on the list of facts.

View your selected facts in the **Report**.



After making your selections, click the **Report** button on the button bar to open your **Reaxys Report**.

Add notes to selected facts in the **Report**.



Click the **Annotation** link on the upper right side of an item to add notes to the selected fact.

Display the structure for a selected fact in the **Report**.



Click the **Show Substance** link to display the substance that goes with the selected fact. The substance will display even though it was not selected with the fact on the results page.

Regroup selected facts in the **Reaxys Report**.



Click the **Regroup** button to reconstruct your report by collecting individual items that were derived from the same record and combining them into one item.

Email the selected facts to a colleague.



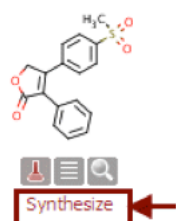
Click the **Send** button to email your comments to colleagues along with your **Reaxys Report** as an attachment to an email.

Export.



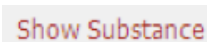
Click the **Output** button and select from several options.

Start a **Synthesis Plan**.



Click the Synthesize link below a substance to start a plan using that substance. Alternatively, you can click the Synthesis Plans button from the button bar and then click the New button in the upper left side of the screen to begin a search from within the Synthesis Planner.

Link to external docs.



Links to **Title/Abstract**, **Full Text**, and View **Citing Articles** appear with references when available.

TOPIC	PAGE
Register for a password .	1
Change password .	1
Find out about tested environments involving Windows, Mac, and Java.	1
Find information about the databases included in a Reaxys search.	1
Select a Structure Editor.	1
Use these external structure editors:	1
<ul style="list-style-type: none"> - Accelrys ISIS/Draw - ChemDraw - Accelrys Draw - ICEdit - CrossFire SE 	
Select Substances or Reactions as the type of search.	2
Create a structure from a name CAS#, InChIkey, or smiles string.	2
Customize the settings for reaction or substance search options .	2
Customize the settings for structure display options.	2
Display a form so that I can use keywords or data in my query.	2
Use the Lookup tables in the Data forms .	3
Customize a Data form .	3-4
Save a Data Form for future use.	4
Add a keyword or data to your query using the Advanced form.	5
Perform Literature Searching .	5-6
Save a query.	6
Set the number of hits per page.	6
Change the structure and text highlight colors.	6
Change the size of substances or reactions .	6
Show/Hide reaction or Substance details.	6
Generate a list of associated reactions from a substance list.	6
Limit results to specific hits.	6
Limit results to hits with specific properties.	7
Limit results to a specific author.	7
View the results from different databases.	7
View a single substance in multiple data-bases.	7
View supplier availability and pricing info.	7
Create an Alert .	7
Save Results .	8
Copy a substance or reaction from the Results screen.	8
Start an AutoPlan .	8
Select the settings for Autoplan .	8

TOPIC	PAGE
Close tabs in the Synthesis Planner .	8
Copy a synthesis plan to the Reaxys Report .	8
Filter using histograms .	8
Select specific details to copy to the Reaxys Report .	9
Select a whole list of details to copy to the Reaxys Report .	9
View your selected facts in the Report .	9
Add notes to selected facts in the Report .	9
Display the structure for a selected fact in the Report .	9
Regroup selected facts in the Reaxys Report .	9
Email the selected facts to a colleague.	9
Export.	9
Start a Synthesis Plan .	9
Link to external docs.	9

